Molecular Insights into the Hydration of Zwitterionic Polymers

Sara A. Tolba [1], and Wenjie Xia [2,3,*]

[1] Materials and Nanotechnology, North Dakota State University, Fargo, North Dakota 58108, United States

[2] Department of Civil, Construction and Environmental Engineering, North Dakota State University, Fargo, North Dakota 58108, United States

[3] Department of Aerospace Engineering, Iowa State University, Ames, Iowa 50011, United States

*Correspondence: wenjie.xia@ndsu.edu, wxia@iastate.edu

Supporting Information

In this work, the water content (WC) of hydrated models is calculated using the following formula:

$$WC = \frac{\rho_{wet} - \rho_{dry}}{\rho_{dry}} * 100\%$$

Such that ρ is the density of the crystal structure and is calculated as follows:

$$\rho = \frac{(Z * M)}{V * N_A}$$

$$V = a * b * c \sqrt{1 - \cos^2(\alpha) - \cos^2(\beta) - \cos^2(\gamma) + 2 * \cos(\alpha)\cos(\beta)\cos(\gamma)}$$

where Z is the number of formula units in the unit cell, M is the molecular weight of the formula unit, V is the volume of the unit cell, N_A is Avogadro's number, a, b, and c are the unit cell parameters, and α, β, and γ are the angles between them.

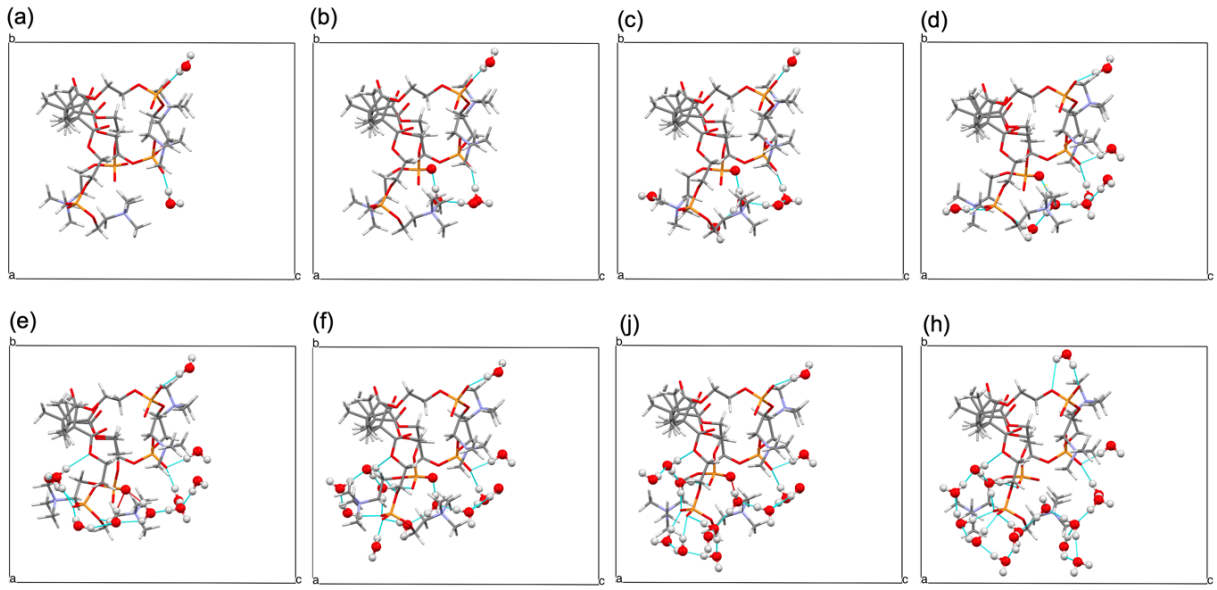

Figure S1. Ground structures of hydrated polyMPC with water content % (WC) of (a) 3.04, (b) 6.10, (c) 9.14, (d) 12.20, (e) 15.23, (f) 18.30, (g) 21.36, and (h) 24.39.

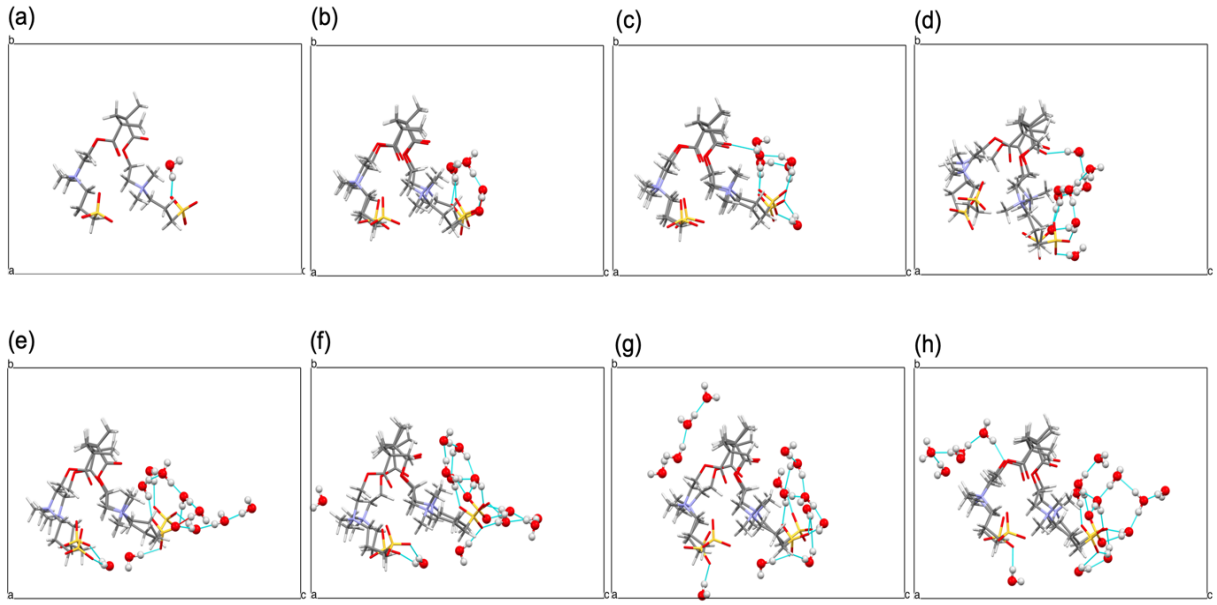

Figure S2. Ground structures of hydrated polySB with water content % (WC) of (a) 3.23, (b) 6.46, (c) 9.68, (d) 12.92, (e) 16.14, (f) 19.37, (g) 22.6, and (h) 25.81.

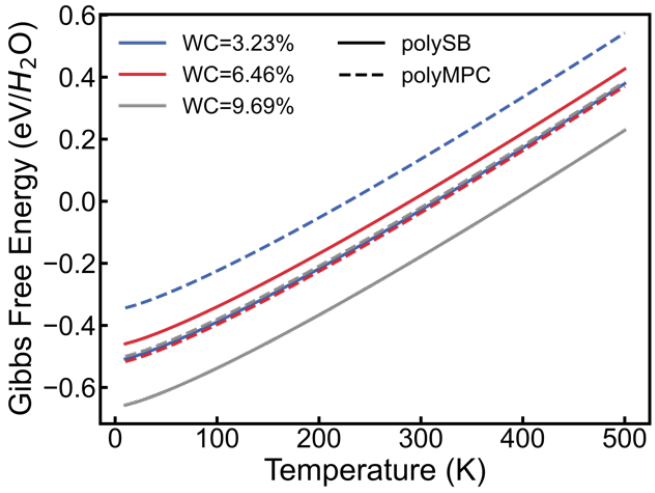

Figure S3. Calculated Gibbs free energy of water adsorption verses temperature for different WC %.

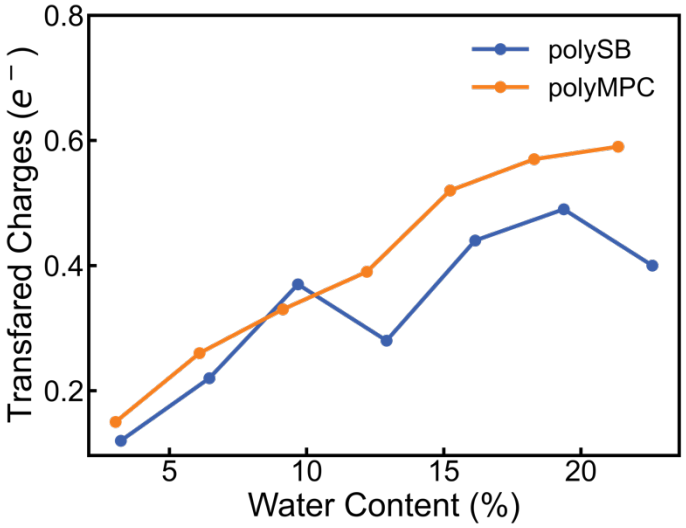

Figure S4. Total charge transferred from polymers to the adsorbed water molecules based on based Löwdin charges.

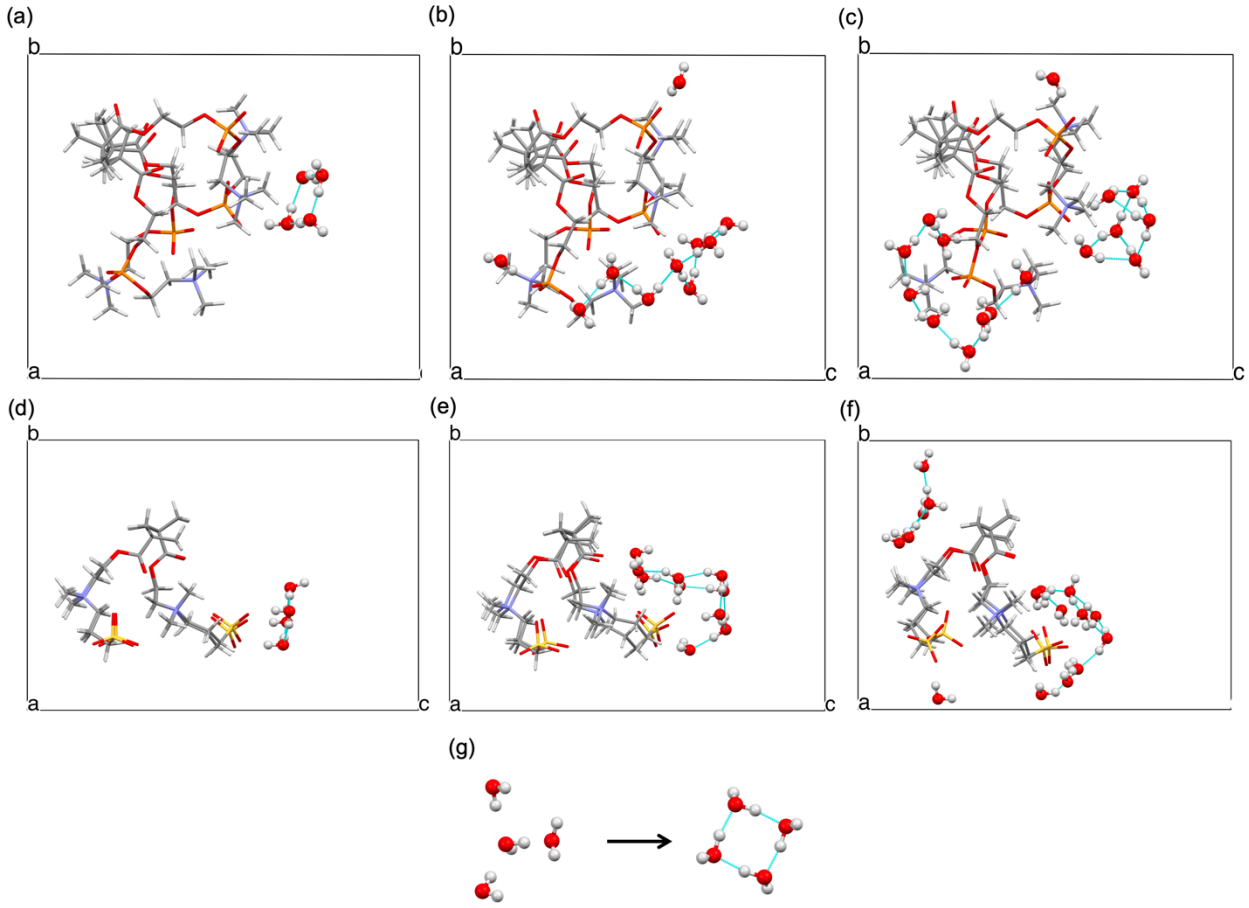

Figure S5. Ground structures of formed small ice cluster on dry (a) polyMPC and (d) polySB. (b)-(c) and (e)-(f) shows the cluster on wet polyMPC and polySB with WC ~ 9.5% and 19.5%, respectively. (g) structural transformation from liquid-like and ice-like water molecules. Red, yellow, Orange, purple, gray, and white atoms are Oxygen, Sulfur, Phosphorus, Nitrogen, Carbon, and Hydrogen, respectively. Dashed cyan line represents hydrogen bonds